

General Disclaimer

One or more of the Following Statements may affect this Document

- This document has been reproduced from the best copy furnished by the organizational source. It is being released in the interest of making available as much information as possible.
- This document may contain data, which exceeds the sheet parameters. It was furnished in this condition by the organizational source and is the best copy available.
- This document may contain tone-on-tone or color graphs, charts and/or pictures, which have been reproduced in black and white.
- This document is paginated as submitted by the original source.
- Portions of this document are not fully legible due to the historical nature of some of the material. However, it is the best reproduction available from the original submission.

(NASA-CR-175485) COMETARY ATMOSPHERES:
MODELING THE SPATIAL DISTRIBUTION OF
OBSERVED NEUTRAL RADICALS Interim Report,
Dec. 1984 - Feb. 1985 (Atmospheric and
Environmental Research) 8 p HC A02/NP A01

N85-21098

G3

91

Unclas

15185

Cometary Atmospheres:

Modeling the Spatial Distribution of Observed Neutral Radicals

Michael R. Combi

Atmospheric and Environmental Research, Inc.

840 Memorial Drive

Cambridge, MA 02139

February 1985

Interim Report for the Period

December 1, 1984 to February 28, 1985

Prepared for

NASA Headquarters

TECHNICAL REPORT STANDARD TITLE PAGE

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.	
4. Title and Subtitle Cometary Atmospheres: Modeling the Spatial Distribution of Observed Neutral Radicals		5. Report Date February 1985	
		6. Performing Organization Code	
7. Author(s) Michael R. Combi		8. Performing Organization Report No.	
9. Performing Organization Name and Address Atmospheric and Environmental Research, Inc. 840 Memorial Drive Cambridge, MA 02139		10. Work Unit No.	
		11. Contract or Grant No. NASW-3950	
12. Sponsoring Agency Name and Address NASA Headquarters Headquarters Contract Division Washington, DC 20546		13. Type of Report and Period Covered Interim Report December 1984-February 1985	
		14. Sponsoring Agency Code	
15. Supplementary Notes			
16. Abstract An algorithm for the random walk problem of multiple elastic collisions between newly formed non-thermal neutral cometary radicals and the outflowing cometary molecules has been incorporated into the Monte Carlo particle-trajectory model. Preliminary model analysis has shown that the effects of collision on the observed spatial distribution of cometary radicals becomes important for the larger bright comets, especially at smaller values of the heliocentric distance. The model and early results are discussed herein.			
17. Key Words (Selected by Author(s)) comets		18. Distribution Statement	
19. Security Classif. (of this report) Unclassified	20. Security Classif. (of this page) Unclassified	21. No. of Pages 7	22. Price*

*For sale by the Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia 22151.

Program of Research in the Third Quarter

During this past quarter, research activities have concentrated on development of the algorithm for including collisions in the Monte Carlo particle-trajectory model.

Multiple Collisions in Cometary Atmospheres

Models of neutral cometary comae have generally dealt with the two extreme cases: one where the densities are high enough so that all neutral species are thermalized and are characterized by a bulk radial flow away from the nucleus, and the other where the densities are so low that essentially no collisions occur. A characteristic distance from the nucleus separating these two regions has been defined where the mean free path for a collision is equal to the distance from the nucleus. Whipple and Huebner (1976), for example, express this collision radius as

$$r_c = \frac{Q\sigma}{4\pi v}$$

where Q = molecular production rate
 σ = cross-section for elastic scattering $\sim 10^{-15} \text{ cm}^2$
 v = molecular outflow velocity.

The value of r_c varies from $\sim 10^4$ km for a bright comet like Kohoutek near perihelion, down to $\sim 10^2$ km for a small short period comet like P/Encke at 1 AU.

In reality, though, there is no clear separation between the two zones. In order for a typical radical (CN, C_2 , OH) which has been emitted from its parent with some exothermic velocity to be truly thermalized, it needs on the order of 10 collisions with outflowing water molecules. On the other hand, many radicals produced outside of r_c will be subjected to at least 1 to 5 collisions, thus questioning the true applicability of a free flow model. What we truly have, then, is a large regime on the order of $0.2 r_c$ to $5 r_c$ where partial thermalization will occur.

The true random walk nature of the elastic scattering problem is modeled in a straightforward manner in the Monte Carlo particle-trajectory model (MCPTM). Kitamura et al. (1983) have included collisions in a Monte Carlo

model essentially based on our original model (Combi and Delsemme 1980a). Since they followed the correct procedure, we have adopted a similar algorithm. There is one problem with their procedure which involves the expression they assume for the density of outflowing molecules with which the modeled neutral radicals are colliding. They assume a Haser-like description for the density which is

$$n_{\text{H}_2\text{O}}(r) = \frac{Q}{4\pi v} \frac{1}{r^2} \exp(-r/v\tau_{\text{H}_2\text{O}})$$

where Q, v are as above

r = distance from the nucleus

$\tau_{\text{H}_2\text{O}}$ = photochemical lifetime for H_2O .

Strictly speaking, this is the correct density distribution for H_2O molecules, but as the H_2O molecules dissociate, they produce OH and H, which still provide targets with which radicals collide. Since the effective cross-sectional area for the fragments is larger than the parent H_2O but their outflow velocity is, on the average, larger, a better approximation would be to simply drop the exponential term in the density expression. This yields

$$n_{\text{H}_2\text{O}}(r) = \frac{Q}{4\pi v r^2}.$$

For the simple case of no radiation pressure, this yields a closed form algebraic expression for the collision length of an arbitrarily moving neutral species, in place of the integral found by Kitamura et al.

The random walk algorithm begins with the production of a neutral radical by its parent with a given velocity vector. From this location and velocity vector, a collision length is given by assumed values for the collision cross section, the molecular (H_2O) production rate, and a random number. The neutral is then displaced this distance, scattered elastically off a moving water molecule and continued on for another collision. The trajectory proceeds this way until the observation time snap-shot.

Preliminary model runs have been performed for the case of CN produced by the photodissociation of HCN (Combi and Delsemme 1980b). We have chosen parameters appropriate for the photochemical lifetimes at 1 AU and have neglected radiation pressure, which is of less importance at 1 AU, for the

purpose of simplifying the preliminary analysis. Subsequent models will test both processes simultaneously. The physical parameters of the coma models are listed in Table 1.

Models were run for cases of general molecular production rates from $1 \times 10^{28} \text{ s}^{-1}$ to $1 \times 10^{30} \text{ s}^{-1}$. The collision statistics from these model runs are summarized in Table 2. As can be seen, for larger gas production rates, only half of the CN radicals produced are in a true free-flow regime. Furthermore, the effect collisions have on the determination of radical production rates is also evident in these model runs. For the case of the largest gas production rate, if one neglects collisions in the model, an underestimate of 11% to 15% in the determination of radical production rate would be made, depending upon the size of the photometer aperture used. The systematic errors, when reducing data for even smaller heliocentric distances ($r_H \sim 0.5 \text{ AU}$), should be quite important in bright comets such as P/Halley, since at these distances the collisional effects are compounded by larger gas production rates and smaller radical parent scale lengths.

Program of Research for the Fourth Quarter

Research efforts in the last quarter will concentrate on (1) model analysis of the effect of collisions on the spatial distributions of the neutral radicals, (2) evaluation of newly published brightness profiles of C_2 (Cochran 1985), (3) incorporation of time dependent production rates and lifetimes into the model code, and (4) preliminary model runs for OH, C_2 and C_3 .

References

- Cochran, A. (1985) *Astrophys. J.* 289, 388.
- Combi, M.R. and A.H. Delsemme (1980a) *Astrophys. J.* 237, 633.
- Combi, M.R. and A.H. Delsemme (1980b) *Astrophys. J.* 237, 641.
- Kitamura, Y., O. Ashihara and T. Yamamoto (1983) *ISAS Research Note* 153.
- Whipple, F.L. and W.F. Huebner (1976) *Ann. Rev. Astron. Astrophys.* 14, 143.

Table 1

CN Radical Coma Model Parameters

$$r_H = 1 \text{ AU}$$

$$\tau(\text{HCN}) = 9 \times 10^4 \text{ s}$$

$$\tau(\text{CN}) = 2.75 \times 10^5 \text{ s}$$

$$v(\text{parent}) = 0.58 \text{ km/s}$$

$$v_e(\text{CN}) = 1.02 \text{ km/s}$$

$$\sigma_{\text{scattering}} = 1 \times 10^{-15} \text{ cm}^{-2}$$

Table 2
Collision Statistics for the CN Model at 1 AU

		Fraction of Radicals Undergoing n Collisions				
Q_{H_2O}	n	0	1-2	3-5	6-10	>10
1×10^{28}		.723	.272	.0042	.0005	.0003
5×10^{28}		.705	.283	.0094	.0023	.0005
1×10^{29}		.681	.296	.0160	.0055	.0009
2×10^{29}		.653	.311	.0247	.0101	.0016
5×10^{29}		.576	.343	.0503	.0252	.0055
1×10^{30}		.503	.355	.0852	.0459	.0147